

Methyl 2-hydroxypropanoate
547-64-8 | DTXSID0027197

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 3.16×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 5.65×10^{-1}

Confidence level: 8.58×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Methyl 2-hydroxypropanoate

Measured: 2.80×10^{-12}

Predicted: 3.16×10^{-12}

Image not found

Ethyl lactate

Measured: 3.90×10^{-12}

Predicted: 4.80×10^{-12}

Image not found

2-Ethoxyethyl acetate

Measured: 1.30×10^{-11}

Predicted: 1.03×10^{-11}

Image not found

Butanoic acid

Measured: 2.40×10^{-12}

Predicted: 2.30×10^{-12}

Image not found

2-Methylpropanoic acid

Measured: 2.00×10^{-12}

Predicted: 1.95×10^{-12}